

Theory of Josephson transport through spintronics nano-structure

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Abstract

We study the Josephson transport through ferromagnetic insulators (FIs) by taking into account its band structure explicitly. In the case of the fully polarized FIs (FPFIs), we found the formation of a π -junction and an atomic-scale 0 - π transition induced by increasing the FI thickness. More remarkably, in the Josephson junction through spin-filter materials such as Eu chalcogenides, the orbital hybridization between the conduction d and the localized f electron gives rise to the π -junction behavior. Such FI-based π -junctions can be used to implement highly-coherent solid-state quantum bits.

Key words: Josephson junction; Spintronics; Ferromagnetic insulator; Quantum bit

1. Introduction

The developing field of superconducting spintronics subsumes many fascinating physical phenomena with potential applications that may complement non-superconducting spintronics devices [1]. In addition there is an increasing interest in the novel properties of junctions of superconductors and magnetic materials [2,3]. One of the most interesting effects is the formation of a Josephson π -junction in superconductor/ferromagnetic-metal/superconductor (S/FM/S) heterostructures [4,5]. In the ground-state phase difference between two coupled superconductors is π instead of 0 as in the ordinary 0 -junctions. In terms of the Josephson relationship

$$I_J = I_C \sin \phi, \quad (1)$$

where ϕ is the phase difference between the two superconductor layers, a transition from the 0 to π states implies a change in sign of the critical current I_C from positive to negative. Physically, such a sign change of I_C is a consequence of a phase change in the pairing wave-function induced in the FM layer due to the proximity effect. The existence of the π -junction in S/FM/S systems has been confirmed in experiment by Ryzanov et al.[6] and Kontos et al.[7].

Recently, quiet qubits consisting of a superconducting loop with a S/FM/S π -junction have been proposed [8,9]. In quiet qubits, a quantum two-level system is spontaneously generated and therefore it is expected to be robust to the decoherence by the fluctuation of the external magnetic field. From the viewpoint of the quantum dissipation, however, S/FM/S junctions are inherently identical with S/N/S junctions (N is a normal nonmagnetic metal). Thus a gapless quasiparticle excitation in

the FM layer is inevitable. This feature gives a strong dissipative or decoherence effect [10]. Therefore the realization of the π -junction *without* a *metallic* interlayer is highly desired for qubit applications [11–14].

In this paper, we investigate the Josephson effect through a ferromagnetic *insulators* (FIs) numerically. Although the π -junction formation in such junctions has been theoretically predicted [15] and subsequently analyzed by use of the quasiclassical Green's function techniques [16,17], a phenomenological δ -function potential have been used in order to model the FI barrier. Then a natural question to ask is can we realize the π -junction in *actual* FIs? Moreover the possibility of the π -junction formation in the *finite* FI-barrier *thickness* case is also an interesting and unresolved problem. In order to resolve above issues, we will formulate a numerical method for the Josephson current through FIs by taking into account the band structure and the finite thickness of FIs explicitly [18]. Then we will show the possibility of the π -junction formation for two important representative FIs in the spintronics field [19,20], i.e., the fully polarized FI (FPFI) (e.g., $\text{La}_2\text{BaCuO}_5$) and the spin-filter materials (e.g., Eu chalcogenides).

2. Model

Let us consider a two-dimensional tight-binding lattice of the S/FI/S junctions as shown in Fig. 1(a). The vector

$$\mathbf{r} = j\mathbf{x} + m\mathbf{y} \quad (2)$$

points to a lattice site, where \mathbf{x} and \mathbf{y} are unit vectors in the x and y directions, respectively. In the y direction, we apply the periodic boundary condition for the number of lattice sites being W . Electronic states in a superconductor are described by the mean-field Hamiltonian,

$$H_{\text{BCS}} = \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}' \in \text{S}} \left(\tilde{c}_{\mathbf{r}}^\dagger \hat{h}_{\mathbf{r}, \mathbf{r}'} \tilde{c}_{\mathbf{r}'} - \bar{\tilde{c}}_{\mathbf{r}} \hat{h}_{\mathbf{r}, \mathbf{r}'}^* \bar{\tilde{c}}_{\mathbf{r}'}^\dagger \right) + \frac{1}{2} \sum_{\mathbf{r} \in \text{S}} \left(\tilde{c}_{\mathbf{r}}^\dagger \hat{\Delta} \bar{\tilde{c}}_{\mathbf{r}}^\dagger - \bar{\tilde{c}}_{\mathbf{r}} \hat{\Delta}^* \tilde{c}_{\mathbf{r}} \right). \quad (3)$$

Here

$$\hat{h}_{\mathbf{r}, \mathbf{r}'} = [-t_s \delta_{|\mathbf{r}-\mathbf{r}'|, 1} + (-\mu_s + 4t_s) \delta_{\mathbf{r}, \mathbf{r}'}] \hat{\sigma}_0, \quad (4)$$

with

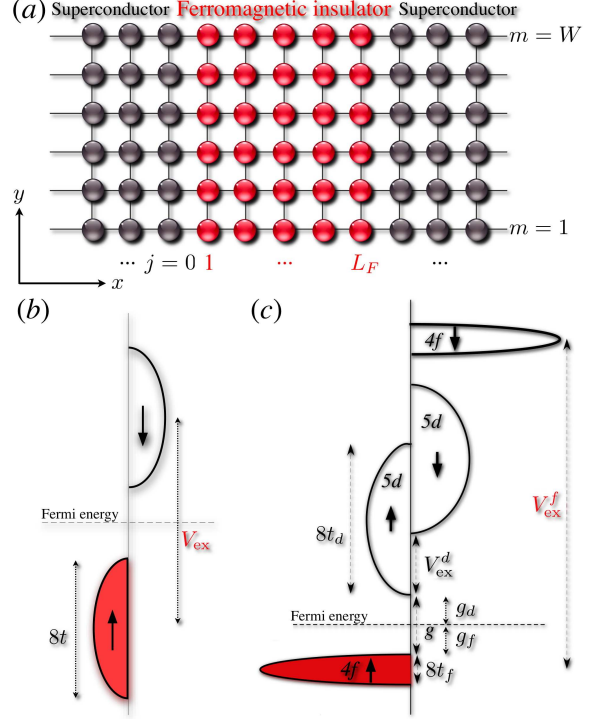


Fig. 1. (Color online) (a) A schematic figure of a Josephson junction through the ferromagnetic insulators on the tight-binding lattice. The density of states for each spin direction for (b) the fully polarized ferromagnetic insulator, e.g., LBCO, and (c) the spin-filter materials, e.g., Eu-chalcogenides.

$$\bar{\tilde{c}}_{\mathbf{r}} = (c_{\mathbf{r}, \uparrow}, c_{\mathbf{r}, \downarrow}), \quad (5)$$

where $c_{\mathbf{r}, \sigma}^\dagger$ ($c_{\mathbf{r}, \sigma}$) is the creation (annihilation) operator of an electron at \mathbf{r} with spin $\sigma = (\uparrow \text{ or } \downarrow)$, $\bar{\tilde{c}}$ means the transpose of \tilde{c} , and $\hat{\sigma}_0$ is 2×2 unit matrix. The chemical potential μ_s is set to be $2t_s$ for superconductors. In superconductors, the hopping integral t_s is considered among nearest neighbor sites and we choose

$$\hat{\Delta} = i\Delta \hat{\sigma}_2, \quad (6)$$

where Δ is the amplitude of the pair potential in the s -wave symmetry channel, and $\hat{\sigma}_2$ is a Pauli matrix.

We consider two representative FIs as a barrier of the Josephson junction, i.e., FPFIs [Fig. 1(b)] and spin-filter materials [Fig. 1(c)]. The typical density of states (DOS) of FPFIs for each spin direction is shown schematically in Fig. 1(b). One of the important FPFIs is $\text{La}_2\text{BaCuO}_5$ (LBCO) [21,22]. The exchange splitting V_{ex} is estimated to be 0.34 eV by a first-principle band calculation [23]. Since V_{ex} is large and the bands are originally half-filled, the system becomes FI.

The Hamiltonian of FPGI layer is described by a single-band tight-binding model as

$$H_{\text{FPGI}} = -t \sum_{\mathbf{r}, \mathbf{r}', \sigma} c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}', \sigma} - \sum_{\mathbf{r}} (4t - \mu) c_{\mathbf{r}, \uparrow}^\dagger c_{\mathbf{r}, \uparrow} + \sum_{\mathbf{r}} (4t - \mu + V_{\text{ex}}) c_{\mathbf{r}, \downarrow}^\dagger c_{\mathbf{r}, \downarrow}, \quad (7)$$

where V_{ex} is the exchange splitting [see Fig. 1(b)]. If $V_{\text{ex}} > 8t$ ($V_{\text{ex}} < 8t$), this Hamiltonian describes FPGI (FM). The chemical potential μ is given by

$$\mu = \frac{V_{\text{ex}}}{2} + 4t. \quad (8)$$

Recently a spin-filter effect has been intensively studied for spintronics applications [19]. Typical spin-filter material is a Eu chalcogenide, e.g., EuO and EuS. The schematic DOS of the Eu chalcogenides is shown in Fig. 1(c). The Eu chalcogenides stand out among the FIs as ideal Heisenberg ferromagnets, with a high magnetic moment and a large exchange splitting of the conduction band for Eu 5d-electrons. Ferromagnetic order of the 4f spins causes exchange splitting of the conduction 5d band, lowering (raising) the spin-up (-down) band symmetrically by $V_{\text{ex}}^d/2$.

For the spin-filter materials such as Eu chalcogenides, we use a following d - f Hamiltonian including the d - f hybridization [24,25],

$$H_{\text{SF}} = H_d + H_f + H_{df}. \quad (9)$$

Here

$$H_d = -t_d \sum_{\mathbf{r}, \mathbf{r}', \sigma} d_{\mathbf{r}, \sigma}^\dagger d_{\mathbf{r}', \sigma} + \sum_{\mathbf{r}} (4t_d - \mu_d) d_{\mathbf{r}, \uparrow}^\dagger d_{\mathbf{r}, \uparrow} + \sum_{\mathbf{r}} (4t_d - \mu_d + V_{\text{ex}}^d) d_{\mathbf{r}, \downarrow}^\dagger d_{\mathbf{r}, \downarrow}, \quad (10)$$

$$H_f = -t_f \sum_{\mathbf{r}, \mathbf{r}', \sigma} f_{\mathbf{r}, \sigma}^\dagger f_{\mathbf{r}', \sigma} + \sum_{\mathbf{r}} (4t_f - \mu_f) f_{\mathbf{r}, \uparrow}^\dagger f_{\mathbf{r}, \uparrow} + \sum_{\mathbf{r}} (4t_f - \mu_f + V_{\text{ex}}^f) f_{\mathbf{r}, \downarrow}^\dagger f_{\mathbf{r}, \downarrow}, \quad (11)$$

$$H_{df} = V_{df} \sum_{\mathbf{r}, \sigma} (d_{\mathbf{r}, \sigma}^\dagger f_{\mathbf{r}, \sigma} + f_{\mathbf{r}, \sigma}^\dagger d_{\mathbf{r}, \sigma}), \quad (12)$$

where $d_{\mathbf{r}, \sigma}^\dagger$ ($f_{\mathbf{r}, \sigma}^\dagger$) is the creation operator, t_d (t_f) is the hopping integral and V_{ex}^d (V_{ex}^f) is the exchange splitting of d (f) electrons. The chemical potential of d and f electrons is respectively given by

$$\mu_d = -g_d \quad (13)$$

$$\mu_f = 8t_f + g_f, \quad (14)$$

where g_d (g_f) is the energy gap of the d (f) band [see Fig. 1(c)]. The third term H_{df} of the Hamiltonian describes the mixing between d and f electrons.

The Hamiltonian is diagonalized by the Bogoliubov transformation and the Bogoliubov-de Gennes equation is numerically solved by the recursive Green function method [26]. We calculate the Matsubara Green function $\check{G}_{\omega_n}(\mathbf{r}, \mathbf{r}')$ in a FI layer,

$$\check{G}_{\omega_n}(\mathbf{r}, \mathbf{r}') = \begin{bmatrix} \hat{g}_{\omega_n}(\mathbf{r}, \mathbf{r}') & \hat{f}_{\omega_n}(\mathbf{r}, \mathbf{r}') \\ -\hat{f}_{\omega_n}^*(\mathbf{r}, \mathbf{r}') & -\hat{g}_{\omega_n}^*(\mathbf{r}, \mathbf{r}') \end{bmatrix}, \quad (15)$$

where

$$\omega_n = (2n + 1)\pi T \quad (16)$$

is the Matsubara frequency. The Josephson current is given by

$$I_J(\phi) = -ietT \sum_{\omega_n} \sum_{m=1}^W \text{Tr} [\check{G}_{\omega_n}(\mathbf{r}', \mathbf{r}) - \check{G}_{\omega_n}(\mathbf{r}, \mathbf{r}')], \quad (17)$$

with T being a temperature and $\mathbf{r}' = \mathbf{r} + \mathbf{x}$. Throughout this paper we fix the following parameters: $W = 25$, and $\Delta_0 = 0.01t$, $T = 0.01T_c$, where T_c is the superconductor transition temperature.

3. Josephson current through FPGI

We first investigate the Josephson transport through FPGIs [Fig. 1(b)]. In the calculation, we assume $t = t_s$ for simplicity. The phase diagram depending on the strength of V_{ex} ($0 \leq V_{\text{ex}}/t \leq 8$ for FM and $V_{\text{ex}}/t > 8$ for FPGI) and L_F is shown in Fig. 2. The black (white) regime corresponds to the π - (0 -)junction, i.e., $I_J = -(+)I_C \sin \phi$. In the case of FPGI, the π -junction can be formed. Moreover remarkably, *the atomic-scale 0 - π transition is induced by increasing the thickness of the FI barrier L_F* . The physical origin of the 0 - π transition will be discussed in elsewhere [27].

4. Josephson current through spin-filter materials

Next we consider the Josephson transport through the spin-filter materials such as the Eu chalcogenides. In the calculation, we use the following parameters in consideration of EuO: $t_d = 1.25$

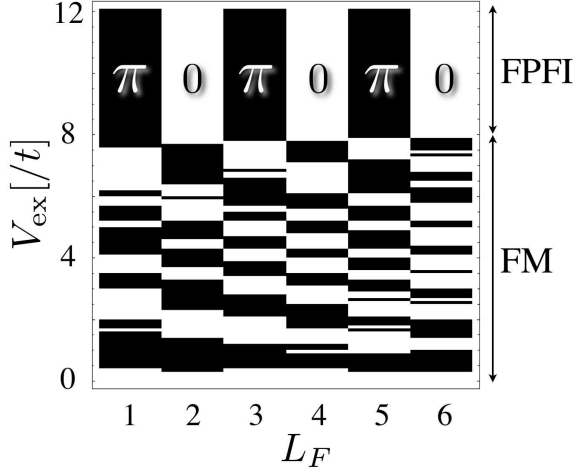


Fig. 2. The 0- π phase diagram depending on the exchange splitting V_{ex} and the thickness L_F for FM ($0 \leq V_{\text{ex}}/t \leq 8$) and the fully polarized FI ($V_{\text{ex}}/t > 8$). The black and white regime correspond to the π - and 0-junction, respectively.

eV, $g_d = 7.5$ eV, $g_f = 0.075$ eV, and $V_{\text{ex}}^d = 0.528$ eV. For simplicity, we assume $t_d = t_s$.

We first discuss the Josephson current through the $5d$ -band only in order to check whether the spin-filter effect gives rise to the π -junction behavior or not. In this case, we numerically found that no π -junction is formed irrespective of the thickness L_F and V_{ex}^d . Therefore the spin-filter effect gives rise to only the 0-junction behavior.

Next we consider the Josephson transport through the Eu-chalcogenides including both the $5d$ - and $4f$ -band. In the calculation we set $L_F = 5$. We systematically change the values of the hopping integral for the f band t_f ($= 0.0 \sim 0.5t_d$) and the d - f hybridization V_{df} ($= 0 \sim 6.5t_d$). Fig. 3 shows the 0- π phase diagram numerically obtained. Remarkably, the π -junction is realized at the certain values of t_f and V_{df} . We found that the π -junction can be formed if (1) d and f band for down spin are overlapped each other (see inset in Fig. 3) and (2) the d - f hybridization V_{df} is strong enough. More detailed discussion for above results will be given in elsewhere [27].

5. Summary

To summarize, we have studied the Josephson effect in S/FI/S junction by use of the recursive Green's function method. We found that the π -junction and the atomic-scale 0- π transition is realized in the case of FPFIs. On the other hand, in the

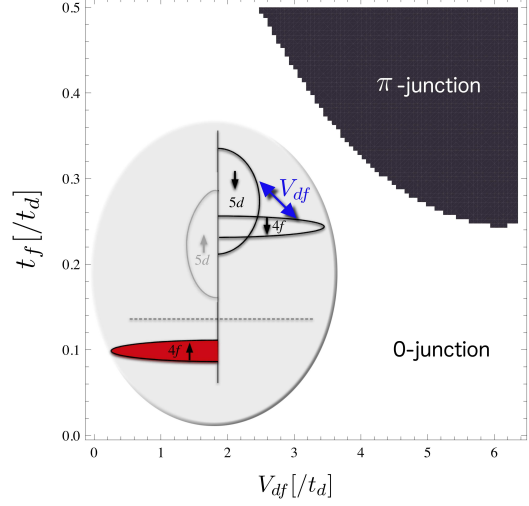


Fig. 3. (Color online) The 0- π phase diagram depending on the d - f hybridization V_{df} and the hopping integral t_f of the f electrons for the Josephson junction through the spin-filter materials. The black and white regime correspond to the π - and 0-junction. Inset shows a schematic DOS configuration for the junction.

case of the Josephson junction with the spin-filter material, the π -junction can be formed if the d and f bands are overlapped and the d - f hybridization is strong. Such FI based π -junctions can be used as an element in the architecture of *ideal quiet qubits* which possess both the quietness and the weak quasiparticle-dissipation nature. Therefore, ultimately, we could realize a FI-based highly-coherent quantum computer.

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References

- [1] I. Zutic, J. Fabian, and S. D. Sarma, Rev. Mod. Phys. **76** (2004) 323.
- [2] A. A. Golubov, M. Y. Kupriyanov, and E. Il'ichev, Rev. Mod. Phys. **76** (2004) 411.
- [3] A. I. Buzdin, Rev. Mod. Phys. **77** (2005) 935.
- [4] L. N. Bulaevskii, V. V. Kuzii, and A. A. Sobyenin, JETP Lett. **25** (1977) 290.
- [5] A. I. Buzdin, L. N. Bulaevskii, and S. V. Panyukov, JETP Lett. **35** (1982) 178.

- [6] V. V. Ryazanov, V. A. Oboznov, A. Y. Rusanov, A. V. Veretennikov, A. A. Golubov, and J. Aarts, *Phys. Rev. Lett.* **86** (2001) 2427.
- [7] T. Kontos, M. Aprili, J. Lesueur, F. Genêt, B. Stephanidis, and R. Boursier, *Phys. Rev. Lett.* **89** (2002) 137007.
- [8] L. B. Ioffe, V. B. Geshkenbein, M. V. Feigel'man, A. L. Fauchère, and G. Blatter, *Nature* **398** (1999) 679.
- [9] G. Blatter, V. B. Geshkenbein, and L. B. Ioffe, *Phys. Rev. B* **63** (2001) 174511.
- [10] G. Schön, and A. D. Zaikin, *Phys. Reports* **198** (1990) 237.
- [11] S. Kawabata, S. Kashiwaya, Y. Asano, and Y. Tanaka, *Physica C* **437-438** (2006) 136.
- [12] S. Kawabata, S. Kashiwaya, Y. Asano, Y. Tanaka, and A. A. Golubov, *Phys. Rev. B* **74** (2006) 180502(R).
- [13] S. Kawabata, and A. A. Golubov, *Physica E* **40** (2007) 386.
- [14] S. Kawabata, Y. Asano, Y. Tanaka, S. Kashiwaya, and A. A. Golubov, *Physica C* **468** (2008) 701.
- [15] Y. Tanaka, and S. Kashiwaya, *Physica C* **274** (1997) 357.
- [16] M. Fogelström, *Phys. Rev. B* **62** (2000) 11812.
- [17] E. Zhao, T. Löfwander, and J. A. Sauls, *Phys. Rev. B* **70** (2004) 134510.
- [18] S. Kawabata, Y. Asano, *Int. J. Mod. Phys. B* **23** (2009) 4320.
- [19] J. S. Moodera, T. S. Santos, and T. Nagahama, *J. Phys. Cond. Mat.* **19** (2007) 165202.
- [20] C. Felser, G. H. Fecher, and B. Balke, *Angew. Chem. Int. Ed.* **46** (2007) 668.
- [21] F. Mizuno, H. Masuda, I. Hirabayashi, S. Tanaka, M. Hasegawa, and U. Mizutani, *Nature* **345** (1990) 788.
- [22] W. Ku, H. Rosner, W. E. Pickett, and R. T. Scalettar, *Phys. Rev. Lett.* **89** (2002) 167204.
- [23] V. Eyert, K. H. Höc, and P. S. Riseborough, *Europhys. Lett.* **31** (1995) 385.
- [24] W. Nolting, *Phys. Stat. Sol. (b)* **96** (1979) 11.
- [25] W. Nolting and A. Ramakanth, *Phys. Rev. B* **33** (1986) 1838.
- [26] Y. Asano, *Phys. Rev. B* **63**, 052512 (2001).
- [27] S. Kawabata, Y. Asano, Y. Tanaka, A. A. Golubov, S. Kashiwaya, *Phys. Rev. Lett.* **104**, 117002 (2010).